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Method for estimating the temperature distribution in a phase change material with a broad phase-change-temperature range

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Abstract

We have conducted this study to find an equation that is capable of predicting the temperature distribution in a semi-infinite phase change material (PCM) that has broad phase-change-temperature range on the condition that the initial temperature distribution is uniform at a lower temperature than the phase-change-temperature, and the surface is kept at a higher temperature than the phase-change-temperature. We found that the temperature distribution in the PCM with broad phase-change-temperature range can be approximated by substituting the lower inflection point temperature of the Gaussian distribution of the apparent specific heat for the phase-change-temperature in the equations that express temperature distribution in the PCM with a specific phase-change-temperature.

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Keywords: PCM ; broad phase-change-temperature range ; amount of stored heat

1. Introduction

Phase change material (PCM) is used as a heat storage material in some buildings such as passive solar houses [1]. In regards to the design and operation of heat storage systems that utilize PCM, it would be useful to estimate the temporal change in the amount of heat stored in the PCM by substituting some physical properties of the PCM and boundary conditions in the equation without running numerical simulation.

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Rigorous or approximate analyses of the heat transmission phenomenon involving melting and solidification have been performed only for a limited number of cases [2]. Some rigorous or approximate analyses have been carried out for cases in which a pure substance was used as the PCM and the phase change occurred at a specific temperature. Unfortunately, no analysis has been conducted on the case in which the phase change occurred throughout the wide temperature. To derive the equation that can predict the temporal change in the amount of heat stored in the PCM that has broad phase-change-temperature, temperature distribution in the PCM has to be expressed by an equation. Therefore, we have conducted this study to find an equation that can predict the temperature distribution in the PCM with a broad phase-change-temperature range.

First, we conducted an experiment to measure the one-dimensional temperature distribution in the PCM with a broad phase-change-temperature range on the condition that the initial temperature distribution was uniform at a temperature lower than the phase-change-temperature, and the surface was kept at a temperature higher than the phase-change-temperature. Next, we devised a numerical simulation method to express the thermal behavior of the PCM with a broad phase-change-temperature range under some conditions including the experimental condition. The validity of the simulation method was verified by comparing the result with the experimental result.

To find the equation that can predict the temperature distribution in the PCM with a broad phase-change-temperature range, we checked the feature of the numerically calculated temperature distribution and investigated the method for utilizing the equation that had been derived for the PCM that has a specific phase-change-temperature.

Nomenclature

C	apparent specific heat, J/kgK
L	latent heat, J/kg
t	time, s
T	temperature, °C
T_1	temperature in liquid region, °C
T_2	temperature in solid region, °C
T_i	initial temperature, °C
T_l	lower inflection point temperature of the Gaussian distribution of the apparent specific heat, °C
T_m	phase change temperature, °C
T_s	surface temperature, °C
x	distance from surface, m
α	thermal diffusivity, m^2/s
λ	thermal conductivity, W/mK
ρ	density, kg/m^3

2. Experimental setup and results

2.1. Experimental setup

We conducted an experiment to measure the one-dimensional temperature distribution in the PCM with a broad phase-change-temperature range on the condition that the initial temperature distribution was uniform at a temperature lower than the phase-change-temperature and the surface was kept at a temperature higher than the phase-change-temperature.

We used paraffin as the PCM. In order to calculate the apparent specific heat of the paraffin, the normalized DSC (Differential Scanning Calorimetry) measured power (in W/g) was divided by the heating rate (°K/s), which resulted in the curves shown in Fig. 1. In Fig. 1, we can see that the phase change occurs over a temperature range.

Fig. 2 shows a schematic diagram of the experimental equipment. Melted PCM was poured in a stainless steel container that with a 350 mm square opening and a depth of 100 mm. Insulation material was installed in the range of 50 mm from the edge of the container to reduce 2-dimensional heat loss. Sheet heaters were installed on the upper surface and the undersurface to control the surface temperature. The temperatures of the sheet heaters were controlled by thermal control units. One-millimeter-thick copper sheets were installed between the PCM and the

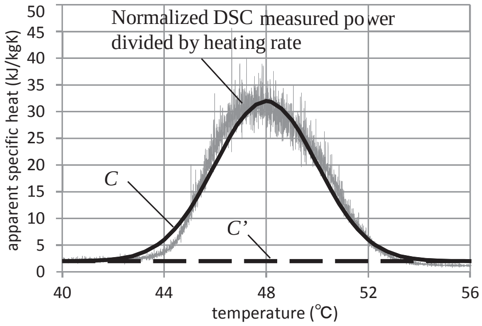

Fig. 1. Apparent specific heat of PCM

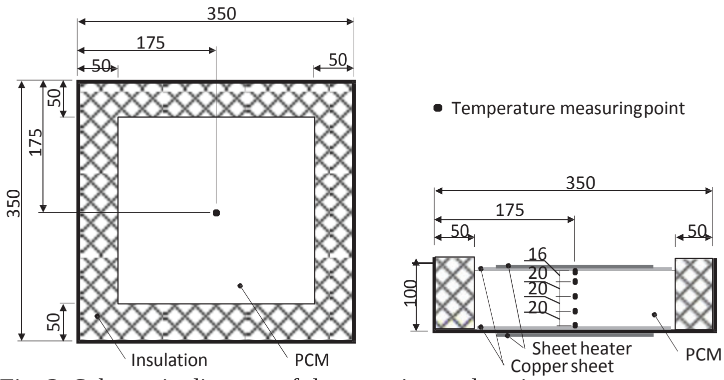

Fig. 2. Schematic diagram of the experimental equipment (Left: plan view, Right: cross-section view) (Unit : mm)

sheet heaters to create a uniform temperature distribution on the upper surface and the undersurface of the PCM. The vertical temperature distribution in the PCM at the center of the square was measured using thermocouples at 0 mm, 16 mm, 36 mm, 56 mm, and 76 mm beneath the upper surface. The recording period was 1 second.

The temperatures of the sheet heaters on the upper surface and the undersurface were kept at 39 °C until the temperature distribution in the PCM became uniform at 39 °C. After that, we increased the temperature of the upper sheet heater to 56 °C. Because the upper surface of the PCM was heated, we assumed that natural convection did not occur in the PCM and heat transferred by conduction only.

2.2. Experimental results

Fig. 3 shows vertical temperature distribution in the PCM at the center of the square at 600, 1200, and 1800 seconds after the time at which we increased the temperature of the upper sheet heater to 56 °C. From this figure, we can see that the temperature in the PCM increases with time.

3. Numerical simulation

3.1. Numerical simulation method

We devised a simulation method for expressing the thermal behavior of the PCM that has broad phase-change-temperature range under some conditions including the experimental condition shown in Chapter 2.

The numerical simulation was conducted by using a forward finite difference method based on the equation for one-dimensional non-steady state heat conduction (Eq. (1)).

$$\rho c \frac{d\theta}{dt} = \lambda \frac{d^2\theta}{dx^2} \tag{1}$$

In the numerical simulation, the time interval was 0.1 s, and the depth interval in the PCM was 1 mm. The results did not change when we used smaller time intervals and smaller depth intervals.

The density and the thermal conductivity of the PCM used in the numerical simulation were 840 kg/m^3 and 0.235 W/mK, respectively. We got these values from the measurements of the PCM we used.

3.2. Apparent specific heat

As seen in Fig. 1, the apparent specific heat between 42 °C and 54 °C was larger than that of the other range, because the PCM state changed from solid to liquid and needed latent heat in this region. We assumed that the specific heat of the PCM in the solid and liquid states were a constant value *C'*. In this case, *C'* was 2 kJ/kgK.

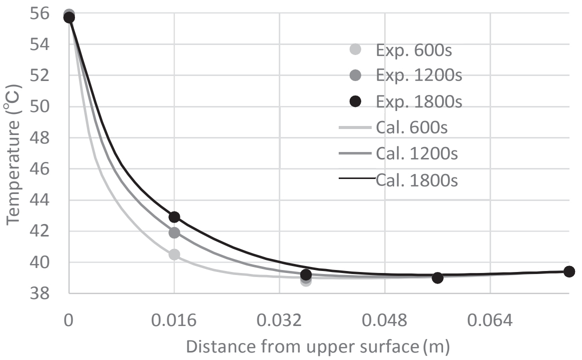

Fig. 3. Vertical temperature distribution in the PCM

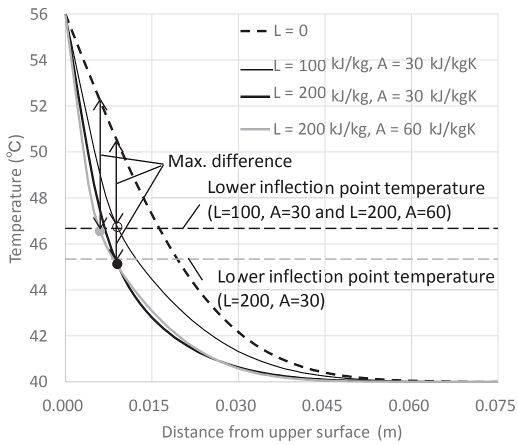

Fig. 4. Temperature distribution in the material that does not include latent heat and temperature distributions in PCM at 1,800 s.

The value obtained by integrating the difference between the apparent specific heat and the value *C'* corresponds to the total quantity of the latent heat *L* of the PCM. In this case, *L* was 150 kJ/kg. We approximated the apparent specific heat shown in Fig. 1 as Gaussian distribution so that the value obtained by integrating the difference between the approximated value and the value *C'* equaled the value *L*. The Gaussian distribution is expressed as Eq. (2).

$$C - C' = A e^{-B(T-T_c)^2}, \qquad B = \frac{A^2 \pi}{L^2} \tag{2}$$

where *C* is the approximated apparent specific heat, *A* is the maximum value of $(C - C')$ and T_c is the central temperature of the Gaussian distribution. In this case, we set *A* as 30 kJ/kgK and T_c at 48 °C.

3.3. Validation of Numerical simulation method

To verify the validity of the numerical simulation method, we compared the result of the simulation with that of the experiment we described in Section 2.

In the numerical simulation, the initial temperature distribution in the PCM was given by linear interpolation of measured temperatures at the measuring points described in Section 2. The measured temperatures of the upper surface and the undersurface were set as boundary conditions.

In Fig. 3, we compare the calculated temperature distribution to the measured temperature distribution. We can see that the calculated temperature distributions are similar to the measured temperature distributions, so the validity of the numerical simulation method is verified.

4. Development of approximate analysis method

Let the material be bounded by the plane $x = 0$ and extend to infinity in the direction of x positive, the initial temperature distribution be uniform at a lower temperature than the phase-change-temperature, and the plane $x = 0$ be kept at a constant temperature that is higher than the phase-change-temperature.

It is assumed that the temperature distribution in the material that includes latent heat (i.e., PCM) is lower than the temperature distribution in the material that does not include latent heat, because latent heat suppresses the temperature rise. Fig. 4 shows the temperature distribution in the material that does not include latent heat and the temperature distributions in the PCM at 1,800 s. The temperature distribution in the material that does not include latent heat is based on Eq. (3), which was derived from the rigorous analysis [3]. The temperature distributions in the PCM were calculated using the numerical simulation method described in Section 3. The values used in these calculations are listed in Table 1 and Table 2.

$$\mathrm{T}(x,t) = T_s - (T_s - T_i)\,\mathrm{erf}\left(\frac{x}{2\sqrt{\kappa t}}\right) \tag{3}$$

Table 1. Values used in calculation (a)

Depth (m)	0.075
Initial temperature (℃)	40
Upper surface temperature (℃)	56
Lower surface temperature (℃)	40

Table 2. Values used in calculation (b)

	material L = 0	PCM
Density (kg/m^3)	840	840
Specific heat (J/kgK)	2500	Eq. (2), *(C'* = 2500)
Thermal conductivity (W/mK)	0.235	0.235
Latent heat (kJ/kg)	0	100, 200
A (max. of C-C') (kJ/kgK)	0	30, 60
Central temp. of Gaussian distribution (℃)	-	48

Though this numerical simulation was conducted for the PCM with a limited depth of 0.075 m, it can be assumed that these results are applicable to the PCM that has semi-infinite depth because the temperatures deeper than approximately 0.06 m did not change from the initial temperature.

In Fig. 4, we also show the points of maximum differences between the temperature in the material that does not include latent heat and the temperatures in the PCM. We can see the depth at which the differences between the temperature in the material that does not include latent heat and the temperatures in the PCM reach their maximum. This depth remains relatively consistent even if there is a difference between the total amount of the latent heat *L* keeping the value of *A*. Furthermore, we can see that at each point, where the temperature difference between the PCM and the material that does not include latent heat reaches its maximum, is almost the same as the lower inflection point temperature of the Gaussian distribution of the apparent specific heat. The lower inflection point temperature of the Gaussian distribution of the apparent specific heat is expressed by Eq. (4).

$$T_l = T_c - \sqrt{\frac{1}{2a}} \tag{4}$$

To find the equation that can predict the temperature distribution in the PCM with a broad phase-change-temperature range, we investigated the method that utilizes some approximate analyses that had already been carried out for the scenario where phase conversion occurs at a specific temperature [2].

Given the case that the initial temperature of the semi-infinite PCM is uniform at T_i and the temperature of the surface is kept at T_s, the temperature distribution in the PCM that has a specific phase-change-temperature T_m is approximately expressed by Eq. (5) and Eq. (6). Equation (5) expresses the temperature distribution in the liquid region, Eq. (6) expresses the temperature distribution in the solid region, and Eq. (7) expresses the position of the solid-liquid interface.

$$T_1(x,t) = T_s - (T_s - T_m)\left\{\mathrm{erf}\left(\frac{x}{2\sqrt{\kappa t}}\right)/\mathrm{erf}(\psi)\right\} \tag{5}$$

$$T_2(x,t) = T_i + (T_m - T_i)\left\{\mathrm{erfc}\left(\frac{x}{2\sqrt{\kappa t}}\right)/\mathrm{erfc}(\psi)\right\} \tag{6}$$

$$X(t) = 2\psi\sqrt{\kappa t} \tag{7}$$

Here,

$$\psi = \frac{1}{2}\left\{-\frac{\beta_2}{\sqrt{\pi}} + \sqrt{2\beta_1 + \left(\frac{\beta_2}{\sqrt{\pi}}\right)^2}\right\}, \quad \beta_1 = \frac{c(T_s - T_m)}{L}, \quad \beta_2 = \frac{c(T_m - T_i)}{L}$$

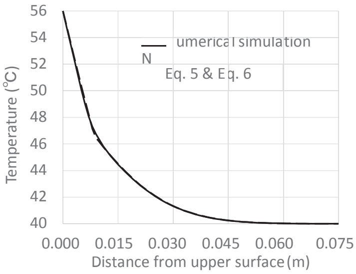

Fig. 5. Temperature distribution (L: 100kJ/kg, A: 30kJ/kgK)

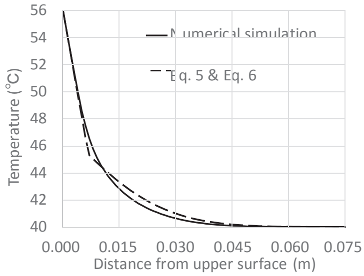

Fig. 6. Temperature distribution (L: 200kJ/kg, A: 30kJ/kgK)

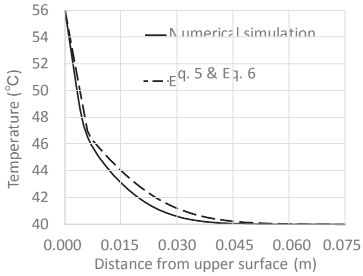

Fig. 7. Temperature distribution (L: 200kJ/kg, A: 60kJ/kgK)

Because much of the heat that flows into the solid-liquid interface is used for phase change, the slope of the temperature distribution at the solid side of the solid-liquid interface is smaller than that of the liquid side. As such, the maximum difference between the temperature in the material that does not include latent heat and the temperature in the PCM with a specific phase-change-temperature occurs at the solid-liquid interface.

By this rationale, we assumed that it may be possible to approximate the temperature distribution in the PCM that has broad phase-change-temperature range by using Eq. (5) and Eq. (6) and by substituting the lower inflection point temperature of the Gaussian distribution of the apparent specific heat for the phase-change-temperature �.

Figs. 5 - 7 show the temperature distribution in the PCM at 1,800 s calculated by the numerical simulation method described in Section 3. These figures also show the temperature distribution in the PCM at 1,800 s calculated by using Eq. (5) and Eq. (6) and by substituting the lower inflection point temperature of the Gaussian distribution of the apparent specific heat for the phase-change-temperature �. The other values used in these calculations are listed in Table 1 and Table 2. The temperature distribution calculated by using the numerical simulation method and the distribution calculated by Eq. (5) and Eq. (6) on the condition L = 100 kJ/kgK and A = 30 kJ/kgK similar to one another. In the other conditions, they are a little less similar. As such, we can see that Eq. (5) and Eq. (6) can approximately express the temperature distribution in the PCM that has broad phase-change-temperature range by substituting the lower inflection point temperature of the Gaussian distribution of the apparent specific heat for the phase-change-temperature.

5. Conclusions

We conducted this study to find an equation that can predict the temperature distribution in a semi-infinite PCM with a broad phase-change-temperature range under the conditions of which the initial temperature distribution is uniform at a temperature lower than the phase-change-temperature and where the surface is kept at a higher temperature than the phase-change-temperature.

We found that it is possible to approximate the temperature distribution in the PCM with a broad phase-change-temperature range by substituting the lower inflection point temperature of the Gaussian distribution of the apparent specific heat for the phase-change-temperature in the equations (i.e., Eq. (5) and Eq. (6)) that express temperature distribution in the PCM with a specific phase-change-temperature.

In this study, we described the possibility that the temperature distribution in the PCM with a broad phase-change-temperature range can be predicted by these equations. However, we need further investigation on the generality and the analytical proof of this method.

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